Solubility of Hydrogen in Heavy n-Alkane Binary Mixtures

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Although most of the available equations of state accurately predict the phase equilibria of simple substances, the situation is different for complex fluids such as polar or chain-like molecules. Since these equations are macroscopic, a systematic modification of them is not possible. On the other hand, equations of state based on molecular theories have proven to be an alternative approach in these cases. In this work we present new experimental measurements on the solubility of hydrogen in several (decane + normal alkane) binary mixtures. Data cover a temperature range from about 315 K up to 450 K, and pressures up to 15 MPa were applied. Hydrogen solubilities of up to 15 mol% were measured. These mixtures are also described through a molecular-based equation of state, and compared with predictions obtained from traditional equations of state. In the SAFT approach all the compounds are modeled as homonuclear chains of united-atom sites interacting through a Lennard-Jones potential. Optimized values for the chain length, Lennard-Jones diameter and dispersive energy characterize the hydrogen molecule. In the case of n-alkanes, a correlation existing in the literature for these molecular parameters is used. Two additional parameters, independent of the thermodynamic variables, are fitted for each particular binary mixture. No further parameters are needed for the ternary systems.